Enter Document Control Number or Bar Code

50010005667

United States Environmental Protection Agency
Washington, DC 20460

Document Description	Date
SAT P01-783	8/22/01

[redacted]

EPA Form 7740-9 (rev. 10/92) Previous edition is obsolete

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98 [redacted]

Case #: P-01-0783	**DCN:**
SAT Date: 8/10/01	**SAT Chair:** B. Jones

Submitter: Solutia Inc.

Chemical Name:

[redacted]

CAS RN: [redacted]	**Trade Name:** SPE 9806

Structure

[redacted]

50010005667

Molecular Formula: [redacted]

Molecular Wt. [redacted]	**WT%<500:**	**WT%<1000:**
MP:	**BP:**	**Eq. Wt:**
H2O Sol (g/L): 1000	**V.P.** <0.000001	
Max. Prod. Volume (kg/yr): [redacted]	**Physical State:** Solid	

USE:

Scale inhibitor, downhole use in oil fields for oil production. [redacted]

Related Case Numbers	Case Role	Related Case Numbers	Case Role
[redacted]		[redacted]	

Focus **Date:** **Results:** 5e Category - Eco, Exposure - based - Health/Eco

STRUCTURE ACTIVITY TEAM REPORT

CASE NUMBER: **P01-0783**

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	2	2

KEYWORDS:

ONCO
BLOOD
DEVEL
NEURO
AQUATOX-A,C

SUMMARY OF ASSESSMENT

FATE: Solid
S (25°C) = 1000 g/L(E); H < 1.00E-8(E)
BP (C) > 400(E); VP @ 25C (mm) < 1.0E-6(E)
POTW removal (%) = 0; Analog data: OECD 306(Biodeg in seawater): 0%/28d; other tests gave little removal over 28d.
Time for complete ultimate aerobic biodeg ≥ mo
PBT Potential: P2B1T2
Sorption to soils/sediments = moderate
*CEB FATE: Migration to ground water = moderate

HEALTH: Absorption is nil through the skin based on physical/chemical properties and good through the lungs and GI tract based on analogs. The PMN material is a chelator although it is already partially chelated [redacted] Because of potential chelating activity, there is concern for neurotoxicity through effects on neuromembranes, effects on blood coagulation, and developmental toxicity [redacted]. There is concern for oncogenicity (bone cancer) by analogy to [redacted]
*CEB HEALTH: Moderate concern (Inhalation and drinking water).
XB: Testing desired (28-day study).

SUBMITTED DATA for free acid or sodium salt:
negative in Salmonella
negative for gene mutations in CHO cells
mouse lymphoma - in vitro study was positive with activation
mouse lymphoma in vitro - negative with and without activation
negative for chromosomal aberration in rat bone marrow cells
range-finding developmental toxicity study in rats - no effects noted at doses up to 2 g/kg

developmental toxicity study in rats (0.5, 1, 2 g/kg) - lower maternal weight gain at 2 g/kg, vertebral anomalies at 1 and 2 g/kg
1-generation reproduction study in rats (300, 1000, 3000 ppm) - reduced number of live pups, increase in dead pups at 3000 ppm; reduced pup weight at 1000 and 3000 ppm; reduced pregnancy rate at 3000 ppm
acute dermal and oral studies
skin and eye irritation studies

On page 21 of the submission, it was noted that there is a carcinogenicity and chronic study for the neutralized acid with a maximum dose of 100 mg/kg with no effects on mineralization of bone, chondral ossification and bone formation/resorption and no changes in neoplastic findings. However this study did not appear to be included in the submission.

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	100.0	P
daphnid 48-h LC50	>	100.0	P
green algal 96-h EC50	=	20.0	P
fish Chronic Value (ChV)	>	10.0	P
daphnid ChV	>	10.0	P
algal ChV	=	2.0	P

based on SAR-nearest analogue method for chelators; SAR chemical class = amine-acid - chelator; [redacted]; hardness <180.0 mg/L as $CaCO_3$, 100% active ingredients, mean measured concentrations, and TOC <2.0 mg/L;
moderate concern for algae only;

assessment factor	=	10.0
concern concentration (CC)	=	0.050

*CEB ECOTOX: All releases to water;

Becky Jones 260-3461

BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0783** Date Received: **8/1/01** Rev. Init: **ACH** OECD Status: **Incomplete** Page: 1 of 15

Genotoxicity data for: [] Submitted Substance [X] Analog: **Various chemicals**

[X]AMES POS/**NEG** (**with**/**without** activation) STRAIN IF (+)

[X]Other: **In the AMES Assay, Dequest 2060 tested negative for gene mutation. In the mouse lymphoma mutation assay, Dequest 2066A and 2060 were negative for gene mutation and clastogenic effects in vitro in the presence or absence of S9-mix. In another mouse lymphoma mutation assay, Dequest 2060 tested positive in vitro, with activation. Dequest 2060, administered via oral gavage, tested negative for chromosomal aberration in rat bone marrow cells. Dequest 2060 tested negative for gene mutations in the CHO cell line.**

Other Data: [X]Ecotox [X]Fate **Biodeg, attachmentW; octanol/water partition coefficient, attachment AA; activated sludge, attachment BB** [X]Water solubility/Log P **Completely soluble, p13** %ai

This information is for: [] Submitted Substance [X] Analog: **Dequest 2066**

Study Type:	**Acute oral**	Study duration:	**14 days**	Species: **Rat**	Sex: **MF**
Wt/Life stage:	**Average males: 210-224 grams, Average females: 133-161 grams/NS**	No. groups/No. per group	**5/10**	Controls: **NS**	
Route:	**Oral**	Dose range:	**5000, 6000, 7000, 8000, 9000 mg/kg**		

Characteristics of tested substance: **NS**

Test Conditions (Dosing Regimen): **A single dose (undiluted) was administered.**

Results: **No mortality was observed. Diarrhea was observed in one animal. Many animals exhibited urine stained fur one day post-dosing. Twenty animals were necropsied at terminal sacrifice. One animal exhibited unilateral hydronephrosis and one animal had a hemorrhagic thymus. The remaining 18 animals were unremarkable. LD50>9000 mg/kg.**

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 2 of 15	
This information is for: [] Submitted Substance	[X] Analog: **SPE 7910**				
Study Type: **Acute oral**	Study duration:	**14 days**	Species: **Rat**	Sex: **MF**	
Wt/Life stage: **150-250 grams/NS**	No. groups/No. per group	**4/4 and 1/10 (high-dose group)**	Controls: **NS**		
Route: **Oral gavage**	Dose range:	**250, 500, 1000, 2000, 5000 mg/kg**			
Characteristics of tested substance: **Brown liquid**					
Test Conditions (Dosing Regimen): **A single dose of the test substance (diluted with distilled water) was administered.**					
Results: **No mortalities or clinical signs of toxicity were observed. All animals showed normal body weight gains at the end of the observation period. No necropsies were performed. LD50>5000 mg/kg.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 3 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2066**				
Study Type: **Acute dermal**	Study duration:	**NS**	Species: **Rabbit**	Sex: **MF**	
Wt/Life stage: **Males: 2.51 kg, Females: 2.52 kg/NS**	No. groups/No. per group	**1/10**	Controls: **Untreated skin**		
Route: **Dermal**	Dose range:	**2000 mg/kg**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied.**					
Results: **No deaths were observed. Erythema was observed in 5 animals. Three animals had necrotic spots on their livers. Two animals had necrotic areas on their hearts. Two animals had kidneys which were pale yellow in color. Five animals were not remarkable. All animals were necropsied at terminal sacrifice. LD50 > 2000 mg/kg.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 4 of 15	
This information is for: [] Submitted Substance	[X] Analog: **SPE 7910**				
Study Type: **Acute dermal**	Study duration:	**14 days**	Species: **Rat**	Sex: **MF**	
Wt/Life stage: **150-250 grams/NS**	No. groups/No. per group	**1/10**	Controls: **Untreated skin**		
Route: **Dermal**	Dose range:	**5 ml/kg**			
Characteristics of tested substance:	**Brown liquid**				
Test Conditions (Dosing Regimen):	**The test article (undiluted) was applied to the shorn skin. A strip of aluminum foil was placed over the treated area and this was held in place with a strip of impermeable adhesive plaster, which was wrapped around the trunk of each animal. After a 24-hour contact period, the wrappings were removed and the treated area was rinsed with warm water.**				
Results:	**No mortalities or signs of toxicity were observed. All animals showed normal body weight gains at the end of the observation period. No necropsies were performed. LD50>5 mL/kg**				

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 5 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2060**				
Study Type: **Eye irritation**	Study duration:	**168 hours**	Species: **Rabbit**	Sex: **NS**	
Wt/Life stage: **NS/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated eye**		
Route: **Eye**	Dose range:	**0.1 mL**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied.**					
Results: **Severe discomfort and thrashing was observed immediately after application. At 10-min post-exposure, necrosis in the conjunctival sac, slight edema, copious discharge, and slight dullness over the cornea were observed. At one-hour post-exposure, no apparent change was observed. At 24-hours post-exposure, very slight to well defined areas of corneal cloudiness, slow iris reaction, necrosis in the conjunctival sac, slight/moderate edema, and copious discharge containing whitish exudate were observed. At 48-168 hours post-exposure, slight improvement was observed. At 14-days post-exposure, slight ulceration in the lower cornea was observed. The test substance was classified as an eye irritant. The average irritation score (24, 48, 72-hour average) was 47.9. The test substance was classified as a severe eye irritant at 24-hours post-exposure.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 6 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2060**				
Study Type: **Eye irritation**	Study duration:	**168 hours**	Species: **Rabbit**	Sex: **NS**	
Wt/Life stage: **NS/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated eye**		
Route: **Eye**	Dose range:	**0.1 mL**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied.**					
Results: **Immediately after exposure, severe discomfort, thrashing, and squealing were observed. One minute after exposure, necrosis in the conjunctival sac was observed. One-hour post-exposure, necrosis in the conjunctival sac, very slight to slight edema, copious discharge, and slight dullness of the cornea were observed. At 24-hours post-exposure, varying degrees of corneal cloudiness, necrosis in the conjunctival sac, very slight to slight edema, and copious discharge containing whitish exudiate were observed. At 48-168 hours post-exposure, gradual slight improvement was observed. The average irritation score (24, 48, and 72-hour average) was 40.8. The test substance was classified as a moderate irritant at one-minute exposure.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 7 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2066**				
Study Type: **Eye irritation**	Study duration:	**72 hours**	Species: **Rabbit**	Sex: **MF**	
Wt/Life stage: **NS/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated eye**		
Route: **Eye**	Dose range:	**0.1 mL**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied.**					
Results: **At 24-hours post-exposure, corneal irritation scores of 5 were assigned to 4/6 animals. Conjunctival irritation scores of 2 were assigned to 2/6 animals. At 48-hours post-exposure, corneal irritation scores of 5 were assigned to 3/6 animals. At 72-hours post-exposure, a conjunctival irritation score of 2 was assigned to 1/6 animals. The average irritation score (24, 48, 72-hour average) was 2.3. The average irritation scores at 24, 48, and 72-hours post-exposure were 4.0, 2.5, and 0.3, respectively.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 8 of 15	
This information is for: [] Submitted Substance	[X] Analog: **SPE 7910**				
Study Type: **Eye irritation**	Study duration:	**7 days**	Species: **Rabbit**	Sex: **NS**	
Wt/Life stage: **2.20-2.38 kg/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated eye**		
Route: **Eye**	Dose range:	**0.1 mL**			
Characteristics of tested substance: **Brown liquid**					
Test Conditions (Dosing Regimen): **The test article was instilled into the conjunctival sac of one eye of each animal. The eyes were not rinsed.**					
Results: **An eye irritation of M1 was obtained. The test substance was classified as a slight irritant. One-day after exposure, redness (score 1) and chemosis (score 1) were observed in 6/6 animals. No other signs of eye irritation observed during the remainder of the study period.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 11 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2066**				
Study Type: **Dermal irritation**	Study duration:	**72 hours**	Species: **Rabbit**	Sex: **MF**	
Wt/Life stage: **NS/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated skin**		
Route: **Dermal**	Dose range:	**0.5 mL**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied to the intact and abraded skin of the test animals.**					
Results: **At 24-hours post-exposure, an erythema score of 1 was assigned to the intact site of 1/6 animals and an erythema score of 1 was assigned to the abraded site of 4/6 animals. No signs of edema were observed at 24-hours post-exposure. At 72-hours post-exposure, an erythema score of 1 was assigned to the abraded skin site of 1/6 animals. Average irritation scores of 0.4 and 0.1 were assigned at 24 and 72 hour observations, respectively. The test substance was classified as a non-irritant.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 12 of 15	
This information is for: [] Submitted Substance	[X] Analog: **SPE 7910**				
Study Type: **Dermal irritation**	Study duration:	**72 hours**	Species: **Rabbit**	Sex: **M**	
Wt/Life stage: **2.52-2.83 kg/NS**	No. groups/No. per group	**1/6**	Controls: **Untreated skin**		
Route: **Dermal**	Dose range:	**0.5 mL**			
Characteristics of tested substance: **Brown liquid**					
Test Conditions (Dosing Regimen): **The undiluted test substance was applied to a gauze pad, which was placed on the shorn intact and abraded skin of the test animals. Cotton wool (approx 1 gram) was placed over the pads. The dressings were secured by a strip of adhesive impermeable plaster, which was wrapped around the trunk of each animal. Twenty-four hours later, the dressings were removed.**					
Results: **Very slight erythema was noted in 4 abraded and 3 intact sites at the 24-hour observation. Three abraded sites also showed very slight edema at that time. All treated skin sites appeared normal at the 72-hour observation. A primary index of 0.4 was obtained. The test substance was classified as a slight skin irritant.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 13 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2061**				
Study Type: **Developmental oral toxicity range-finder**	Study duration:	**17 days**	Species: **Rat**	Sex: **F**	
Wt/Life stage: **Day 3 (carcass weight w/o gravid uterus): 213.2-231.3 grams/NS**	No. groups/No. per group	**2/4 (250 mg/kg, 2 g/kg); 3/5 (100 mg/kg, 500 mg/kg, 1 g/kg); 1/6 (control)**	Controls: **1/6**		
Route: **Oral gavage**	Dose range:	**100, 250, 500 mg/kg; 1, 2 g/kg**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **Animals were dosed via oral gavage on gestation days 6-19.**					
Results: **No mortality was observed. No significant treatment-related effects on body weight, or pre- or post-implantation loss were observed. No treatment-related lesions were observed during gross necropsy of the dams. The only possible treatment-related effect observed in this study was lower body weight gain in the 2 g/kg dose level group. According to the authors, the test material appeared to be relatively non-toxic to pregnant dams, embryos, and fetus, up to dose levels of 2 g/kg.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 14 of 15	
This information is for: [] Submitted Substance	[X] Analog: **Dequest 2061**				
Study Type: **Developmental toxicity-oral**	Study duration:	**17 days**	Species: **Rat**	Sex: **F**	
Wt/Life stage: **Day 3 (carcass weight w/o gravid uterus): 211.0-214.0 grams/NS**	No. groups/No. per group	**2/19 (control and 2 g/kg); 1/17 (0.5 g/kg); 1/21 (1 g/kg)**	Controls: **1/19**		
Route: **Oral gavage**	Dose range:	**0.5 g/kg, 1 g/kg, 2 g/kg**			
Characteristics of tested substance: **NS**					
Test Conditions (Dosing Regimen): **Animals were dosed via oral gavage on gestation days 6-19.**					
Results: **Lower body weight gain and soft stool were observed in the high-dose group. No deaths prior to sacrifice or treatment-related lesions detectable at gross necropsy were observed. No statistically significant treatment-related effects on post-implantation loss or fetus weight were observed. Vertebral anomalies (not statistically significant) were observed in 2 litters of the 2 g/kg group and in one litter of the 1 g/kg group. No treatment-related malformations or variations were observed in the 0.5 g/kg group fetuses.**					

BIOLOGICAL TEST INFORMATION					
Case Number: **P-01-0783**	Date Received: **8/1/01**	Rev. Init: **ACH**	OECD Status: **Incomplete**	Page: 15 of 15	
This information is for: [] Submitted Substance	[X] Analog: **CP 66257**				
Study Type: **Reproductive toxicity**	Study duration:	**1 generation**	Species: **Rat**	Sex: **F**	
Wt/Life stage: **approx 239-241 grams/15-16 weeks**	No. groups/No. per group	**1/35 (controls), 2/19 (300 and 3000 ppm), 1/17 (1000 ppm)**	Controls: **1/35**		
Route: **Oral-diet**	Dose range:	**300, 1000, 3000 ppm**			
Characteristics of tested substance: **Brown, viscous liquid**					
Test Conditions (Dosing Regimen): **Test animals were administered the test chemical in the diet throughout gestation and lactation. Dietary administration of the test chemical continued to the F1 generation animals (10 males and 20 females/group) through a growth period and mating, gestation and lactation period for two successive litters.**					
Results: **In the F0 generation, no treatment effects in the low- or mid-dose groups were evident. In the high-dose group, females delivered litters containing fewer live pups and more dead pups. Pups also had a lower weight at birth. In the F1 generation, no treatment effects were evident in the low-dose group. In the mid-dose group, pup weight at birth was lower than control in the first litters only. In the high-dose group, females had a lower pregnancy rate and delivered smaller pups in the first litters only. No such effects were observed in the second litters and no other treatment-related effects were observed during the remainder of the study. Post-mortem observations and evaluation of selected tissues from 5 adult F1 generation males and females of the control and high-dose group indicated no treatment-related findings.**					

NCSAB SAT REPORT	Submitter	Solutia Inc.	CBI? (Y/N):
PMN P-01-0783	CAS RN [redacted]		Analogs [redacted]
Chem.Name [redacted]			PV(kg) [redacted]

Structure

[redacted]

Scale inhibitor, downhole use in oil fields for oil production.

[redacted]

Formula [redacted]			Eq Wt	
MW [redacted]			Wt%<500	Wt%<1000
MP (M)	MP (E)	BP (M)	BP (E)	VP(E) <0.000001
WS g/L (E) 1000	WS g/L (M)	State Solid		Log P(M)

Endpoint (mg/L)	Est. Value	Meas. Value	Comments	Log P(Epi)
Fish 96-h	> 100			Log P(ClogP)
Daphnid 48-h	> 100			
Algal 96-h	5.0		chelator	
Fish ChV	> 10			
Daphnid ChV	> 10			
Algal ChV	0.50			
BCF				

CHEMICAL CLASS:	SAR: [redacted]; chelator
ECOTOX CONCERN H (M) L	CONCERN CONCENTRATION 0.050
CRSS DATE: 8/9/2001	ASSESSOR:

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 8/10/01

	ATTENDEES	SIGNATURE
	CHEMISTRY	
✓	Paul Bickart	Paul Bickart
	Diana Darling	
✓	Rich Engler	Richard E Engler
	Greg Fritz	
	Daniel Lin	
✓	Kathy Schechter	Kathy Schechter
	ENVIRONMENTAL FATE	
	Bob Boethling	
	David Lynch	
	Gary Thom	
	HEALTH	
✓	Katherine Anitole	Katherine Anitole
✓	Michael Cimino	Michael Cimino
✓	Leonard Keifer	Leonard Keifer
	David Lai	
	Jim Murphy	
	Deborah Norris	
	Ronald Ward	
✓	Yin Tak Woo	Yin Tak Woo
	ENVIRONMENTAL EFFECTS	
	Gordon Cash	
	Vince Nabholz	
✓	Maggie Wilson	Maggie Wilson
	SAT CHAIRPERSON/OTHER	
✓	Rebecca Jones	Rebecca Jones
	Leonard Keifer	
	Vince Nabholz	